

How much complementarity?

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Abstract. Bohr placed complementary bases at the mathematical centre point of his view of quantum mechanics. On the technical side then my question translates into that of classifying complex Hadamard matrices. Recent work (with Barros e Sá) shows that the answer depends heavily on the prime number decomposition of the dimension of the Hilbert space. By implication so does the geometry of quantum state space.

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READING BOHR

Reading what Bohr actually wrote about the foundations of quantum mechanics one is struck by the modesty of his aims [1]. To Bohr, the aim of the theory is to predict the outcomes of measurements performed on a suitably prepared system. In a possibly double edged endorsement of Bohr's position, Mermin stresses how suitable he finds this view when teaching quantum mechanics to students coming from computer science: they want input and output, and have no emotional attachment to what goes on in between [2]. This clearly represents a retreat from the natural position of the physicists, who used to think that the essence of the phenomena resides there—and were then explicitly told by Bohr not to try to disclose them. If Bohr solved the interpretational problem of quantum mechanics then—as Marcus Appleby told me one fine day in front of the Rosetta stone—the problem is to find a point of view from which this solution appears desirable.

It is striking too how little of the mathematical formalism Bohr brings up. The one mathematical point stressed by him is the occurrence, in quantum mechanics, of complementary pairs of measurements: if the system has been prepared to give a definite answer for one of them, nothing is known about the outcome should the complementary measurement be made [1]. Bohr's choice here shows good judgment. It may not be an ideal starting point for axiomatic reconstructions of the theory, but certainly the whole structure can be made to flow naturally through there—as Schwinger so convincingly demonstrated [3]. So Bohr's vision cannot be dismissed lightly.

At this point the discussion can go in many directions, philosophical and technical. The former may be more urgent [4], but my very modest aim here is to discuss how much freedom one has in choosing the complementary measurement. Because of the unitary symmetry the answer is independent of the choice of the first measurement, but it will turn out to depend in an interesting way on which Hilbert space we are in.

COMPLEMENTARY PAIRS OF BASES

Let us assume that the dimension of our Hilbert space is N . We will have to come back to the question what this means. Meanwhile we associate measurements to orthonormal bases in the familiar way. If two such measurements are complementary it must be true that the pair of orthonormal bases $\{|e_i\rangle\}_{i=0}^{N-1}$ and $\{|f_i\rangle\}_{i=0}^{N-1}$ are related by

$$|\langle e_i | f_j \rangle|^2 = \frac{1}{N} \quad (1)$$

for all the basis vectors. The question now arises whether complementary pairs of bases exist in every dimension, and if so how many such pairs exist, counting them up to the natural equivalence under unitary transformations [5].

This problem is equivalent to another that has been studied for a long time. Let us form a matrix with elements

$$H_{ij} = \langle e_i | f_j \rangle. \quad (2)$$

If the two bases are complementary this is a complex Hadamard matrix, that is a unitary matrix all of whose elements have the same modulus. In this way the existence of a complementary pair is equivalent to the existence of a complex Hadamard matrix. It is natural to use one of the members of the pair as our computational basis, in which case the columns of the Hadamard matrix are given by the elements of the vectors in the second basis. Of course we are not interested in the order or the overall phases of these vectors, so we will regard two unitary matrices H' and H as equivalent if there exists a permutation P and a diagonal unitary D such that

$$H' = HDP. \quad (3)$$

But there is still some freedom in the choice of the coordinate system. Given a pair of bases represented by the unit matrix and an Hadamard matrix H , an overall unitary transformation (from the left) with a permutation and a diagonal unitary can be undone from the right when it acts on the unit matrix, while any Hadamard matrix H becomes a new Hadamard matrix H' . So in classifying pairs of complementary bases up to unitary transformations we will regard two complex Hadamard matrices as equivalent if there exist diagonal unitaries D_1, D_2 and permutation matrices P_1, P_2 such that

$$H' = P_1 D_1 H D_2 P_2. \quad (4)$$

If this is so we say that H and H' are equivalent, written $H \approx H'$ [6]. The problem of classifying all complementary bases up to overall unitary transformations is equivalent to classifying all complex Hadamard matrices up to this equivalence. (Classifying all triples of mutually complementary bases is a more involved affair, since the freedom of multiplying from the left will be restricted.) We can remove some of the ambiguity by insisting that all Hadamard matrices should be presented in dephased form, meaning that all entries in the first row and the first column equal $1/\sqrt{N}$.

A complex Hadamard matrix of any size exists. A solution is the Fourier matrix F_N , with entries that are roots of unity only:

$$F_{ij} = \frac{1}{\sqrt{N}} \omega^{ij}, \quad \omega = e^{\frac{2\pi i}{N}}, \quad 0 \leq i, j < N-1. \quad (5)$$

And indeed this is a matrix with many applications. But are there other solutions? It is known that a generic unitary matrix is determined by the moduli of its matrix elements up to the $2N-1$ phases that are removed by dephasing [7], so if the answer is “yes” then Hadamard matrices are quite exceptional among the unitaries.

Our question has a long history. In 1867 the British mathematician Sylvester gave many examples of such matrices [8]. Sylvester also proved uniqueness for $N=2, 3$. In 1893 the French mathematician Hadamard studied the case $N=4$ [9], and found that any Hadamard matrix of this size is equivalent to

$$H(z) = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & z & -1 & -z \\ 1 & -1 & 1 & -1 \\ 1 & -z & -1 & z \end{pmatrix} \approx \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & z & -z \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -z & z \end{pmatrix}. \quad (6)$$

This is a one parameter family of dephased Hadamard matrices, since the phase factor z is arbitrary and invariant (apart from its sign) under the transformations introduced in eq. (4). In 1997 the Danish mathematician Haagerup proved that for $N=5$ the Fourier matrix is again unique up to the natural equivalence [6]. The $N=6$ case is still open. An elegant family of dephased $N=6$ Hadamard matrices with three real parameters was found by Karlsson [10], and there is strong evidence that a four parameter family should exist [11, 12]. Perhaps it has Karlsson’s 3-dimensional family as its boundary? An isolated example not belonging to any continuous family is also known [13]. Finally there are many constructions available in higher dimensions, but we are not even close to a classification [14].

The motivations behind these works were various. Sylvester’s is a very joyful paper written when the notion of a matrix was new, and he was interested in all sorts of patterns he could observe in them. Haagerup’s motivations stemmed from operator algebra. Other motivations for the study of complex Hadamard matrices come from quantum groups [15], and from various corners of quantum information theory [16, 17]. The work on $N=6$ is largely inspired by the problem of Mutually Unbiased Bases in quantum theory, to which we will return. It is worth mentioning that the action of a complex Hadamard matrix can be implemented in the laboratory by means of linear optics [18], and that the $N=6$ case is realistically within reach.

It is intriguing that the answer to the question seems to depend so intricately on the dimension of Hilbert space, but one also wonders if it is at all possible to say something in general about a classification problem that moves this

slowly. I will argue that one can, but first we should see what the existence of complementary pairs means for the geometry of quantum state space.

THE GEOMETRY OF STATE SPACE

Mathematically a quantum state is represented by a density matrix ρ , that is an $N \times N$ complex matrix with non-negative eigenvalues. The set of all quantum states is a compact body of $N^2 - 1$ dimensions, with the pure states $\rho = |\psi\rangle\langle\psi|$ lying at its boundary. The distance D between two density matrices is conveniently defined by

$$D^2(\rho_1, \rho_2) = \frac{1}{2} \text{Tr}(\rho_1 - \rho_2)^2. \quad (7)$$

If we choose the maximally mixed state as the origin we can think of the container space as a real vector space, with the notion of distance coming from the scalar product

$$\rho_1 \cdot \rho_2 = \frac{1}{2} \text{Tr}(\rho_1 - \frac{1}{N} \mathbf{1})(\rho_2 - \frac{1}{N} \mathbf{1}). \quad (8)$$

All the pure states lie on a sphere centered at the maximally mixed state. This sphere is called the outsphere, and the maximally mixed state will be chosen as the origin. An arbitrary state is formed as a mixture of pure states, and it follows that the set of all quantum states forms a convex body with an intricate shape. The reason why the shape is intricate is that the symmetry group of the body is a small but continuous subgroup of the set of all rotations in $N^2 - 1$ dimensions—namely, if we ignore some discrete symmetries, the unitary group or more precisely the group $SU(N)/Z_N$. The pure states therefore form a small but continuous subset of the body's outsphere. We define the insphere as the largest sphere one can inscribe in the body. It is concentric with the outsphere, and the radius of the outsphere is $N - 1$ times the radius of the insphere. (And we learn that the case $N = 2$ is special.)

In order to get a feeling for what the shape is, one can ask what kind of regular polytopes, and similar understandable structures, one can inscribe in it. Indeed an orthonormal basis in Hilbert space corresponds to a regular simplex with N vertices, inscribed in the body of all states, centred at the origin, and spanning a plane through the centre of dimension $N - 1$. Every state ρ lies in a simplex of this type. A complementary pair of bases spans two planes oriented with respect to each other in a special way. In fact the two planes are totally orthogonal, meaning that any vector in one of them is orthogonal to any vector in the other. Note that the totally orthogonal planes already point to the use complementary measurements have in quantum state tomography; other things being equal complementarity will minimize the uncertainties caused by the fact that, in a laboratory with access to a potentially infinite ensemble of identically prepared systems, only a finite number of measurement will actually be carried out [19].

Once we have found a pair of simplices coming from a complementary pair, we can adjust the coordinates so that one basis is described by the computational basis, and then move the other simplex around by acting on the pair from the left with permutations and diagonal unitaries—operations whose action on the computational basis can be undone by irrelevant action from the right with the same type of unitaries. See eq. (4). So there is some freedom, but there will be more freedom the larger the set of inequivalent Hadamard matrices is found to be. The bottom line is that the existence of complementary pairs of bases is very much a question of the shape of the body of density matrices.

We can go on in this way. Since $(N - 1)(N + 1) = N^2 - 1$ we can find $N + 1$ totally orthogonal planes in our $(N^2 - 1)$ -dimensional vector space. We can place a regular simplex of the appropriate size in each plane, but it is not at all clear that its corners correspond to pure states. By construction they lie on the outsphere, but they may well lie well outside the body of states, whose shape is so difficult to discern. But then again it may be possible to inscribe all these simplices in the body, in which case we say that we have a complete system of $N + 1$ Mutually Unbiased Bases [19]—and we have one more handle on the shape.

After many trials in six dimensions [20, 21, 22, 23, 24], most investigators are convinced that complete systems of MUBs exist if—this much is known [19]—and only if—this is a conjecture only—the dimension of the Hilbert space is a power of a prime number. We will not be concerned with this problem here, but it does hang in the background. By the way the best known complete systems of MUBs [19] can be obtained by choosing one special complex Hadamard matrix, and then multiplying it from the left by appropriate permutations and diagonal unitaries to construct the remaining $N - 1$ complementary bases. I would be interested to know if this is true also for the more exotic examples that are known in some prime power dimensions [25], but I don't.

Of course the shape of the body of states can be studied in many other ways. But we are focussing on an important aspect of it.

FAMILIES OF HADAMARD MATRICES

Now let us consider the family of inequivalent Hadamard matrices given in eq. (6). By inspection we see that it includes the Fourier matrix (at $z = i$), but it also includes a real Hadamard matrix (at $z = 1$). The latter has an interesting form: it is the tensor product $F_2 \otimes F_2$. On reflection we realise that whenever the dimension of Hilbert space is composite we can form Hadamard matrices from a pair of Hadamard matrices of size N_1 and N_2 in this way. But it will not always be true that $F_{N_1} \otimes F_{N_2}$ is inequivalent to $F_{N_1 N_2}$. As a matter of fact they are equivalent if and only if N_1 and N_2 are relatively prime. This follows from some elementary group theory, because any Fourier matrix can be regarded as the character table of a cyclic group, and the cyclic group $Z_{N_1 N_2}$ is isomorphic to the cyclic group $Z_{N_1} \times Z_{N_2}$ if and only if N_1 and N_2 are relatively prime. In prime power dimensions it is $F_p \otimes \dots \otimes F_p$, and not the inequivalent matrix F_{p^k} , that lays the golden eggs (i.e., a complete set of MUBs [19]).

There exists a construction due, in its most general form, to Diță [26], allowing us to construct a continuous family in dimension $N = N_1 N_2$ starting from one Hadamard matrix $H^{(0)}$ in dimension N_1 and N_1 possibly different Hadamard matrices $H^{(1)}, \dots, H^{(N_1)}$ in dimension N_2 . It uses a warped tensor product. In dephased form

$$H = \begin{pmatrix} H_{0,0}^{(0)} H^{(1)} & H_{0,1}^{(0)} D^{(1)} H^{(2)} & \dots & H_{0,N_1-1}^{(0)} D^{(N_1-1)} H^{(N_1)} \\ \vdots & \vdots & & \vdots \\ H_{N_1-1,0}^{(0)} H^{(1)} & H_{N_1-1,1}^{(0)} D^{(1)} H^{(2)} & \dots & H_{N_1-1,N_1-1}^{(0)} D^{(N_1-1)} H^{(N_1)} \end{pmatrix} \quad (9)$$

where $D^{(1)}, \dots, D^{(N_1-1)}$ are diagonal unitary matrices (with their first entries equal to one in order to obtain H in dephased form). In this way the example of $N = 4$ generalises. It can be shown that the family arising from the Diță construction using Fourier matrices as seeds interpolates between the non-equivalent matrices F_{n^k} and $F_n \otimes \dots \otimes F_n$ for all values of n [27]. This somehow provides the beginning of a rationale for the existence of this family.

Assuming that the parameters that may be present in the individual $H^{(i)}$ do not complicate matters, the intrinsic topology of these families—if we ignore some discrete equivalences, whose action has been completely worked out only in special cases [20]—is that of a higher dimensional torus. They are examples of the more general class of affine families [14], in which all relations between the phases in the matrix are linear. But affine families are not the end of the story. For $N = 6$ we obtain affine families of at most 2 dimensions, while the set of all inequivalent Hadamard matrices has at least 3, and almost certainly 4, parameters. Moreover Karlsson's 3-dimensional family, which is known in explicit form, has a much more interesting geometry than the tori. Before all the discrete equivalences are taken into account it looks much like a circle bundle over a sphere, but with special points over (some copies of) the Fourier matrix, where the circles are blown up to tori.

ALL HADAMARD MATRICES CONNECTED TO THE FOURIER MATRIX

To address the classification in general we first lower our aim a bit. Rather than ask for all complex Hadamard matrices, we ask for all smooth families of Hadamard matrices that include the Fourier matrix. This is really a question about the dimension of some algebraic variety. Following Fermi—"when in doubt, expand in a power series"—we attack it by multiplying the matrix elements in the Fourier matrix by arbitrary phase factors, which are then expanded in a series:

$$F_{ij} \rightarrow F_{ij} e^{i\phi_{ij}} = F_{ij} \left(1 + i\phi_{ij} - \frac{1}{2}\phi_{ij}^2 + \dots \right). \quad (10)$$

Then we try to solve the unitarity conditions order by order in the free phases ϕ_{ij} , and count the number d of free parameters that remain. To first order in the perturbation Tadej and Życzkowski [14] made this calculation. For dimension N they found the answer

$$D_1 = \sum_{n=0}^{N-1} \gcd(n, N), \quad (11)$$

where $\gcd(n, N)$ denotes the greatest common divisor of n and N . Subtracting $2N - 1$, that is the number of trivial phases arising from eq. (4), this gives an upper bound on the number of free parameters in a smooth family of dephased Hadamard matrices containing the Fourier matrix. If N is a prime this upper bound equals zero, so that we know that

the Fourier matrix is isolated in the set of all Hadamard matrices. If N is a power of a prime the upper bound is equal to the dimension of the family that arises from the Diţă construction, so that this family is the largest possible such family in this case. We tried to see what happens in the remaining cases.

By now my question has become very technical, and for the details I have to refer to a paper by Barros e Sá and myself [27]. In outline, our first step was to use the special properties of the Fourier matrix to write the equations in a more manageable form—in effect we calculate all bases complementary to the Fourier basis, rather than those complementary to the computational basis. To first order in the perturbation the equations are linear and homogeneous, and we recover eq. (11) in a very transparent way. To higher orders we still have to solve a linear system, but now with a heterogeneous part given by the lower order solution. To a given order s these systems have solutions if and only if the lower order solutions obey consistency conditions which take the form of a set of multivariate polynomial equations of order s . If these conditions are non-trivial the true dimension drops below the first order result (11). Should this happen we have to solve the polynomial equations in order to determine by how much the dimension drops, and then we can proceed to higher orders ...

Using a mixture of numerical and symbolical calculations we were able to carry through this program to quite high orders, for 24 different choices of N not equal to a prime power. One case then stands out as being very special: $N = 6$, for which the consistency conditions hold trivially up to order 25 in the perturbation. At order 26 Mathematica quite reasonably refused to continue the calculation. Still, this gives considerable support to the conjecture that a 4-dimensional family of dephased Hadamard matrices does exist in this case—and it warns us not to make induction from six to arbitrary composite dimensions. $N = 10$ also stands out as somewhat special (the consistency conditions break down at order 11). In all other cases the consistency conditions break down in a systematic manner: at order 3 if N is a product of three different primes, at order 4 if N is a product of two different primes, at least one repeated, at order 5 if N is a product of two odd primes, and at order 7 if N is a twice an odd prime and larger than ten.

We looked at the comparatively manageable cases of $N = 12, 18, 20$ in more detail. We found solutions to the consistency conditions in symbolic form. For $N = 12$ we found the general solution to the consistency conditions at order 4, as well as an almost watertight argument saying that there does exist a two-sheeted solution such that no further breakdowns occur in higher orders. This was confirmed up to order 11 by an explicit calculation. Based on this information we conjecture that whenever $N = p_1 p_2^2$, where p_1, p_2 are primes, there will be a non-linear family of dephased complex Hadamard matrices of dimension

$$d = 3p_1 p_2^2 - 3p_1 p_2 - 2p_2^2 + p_2 + 1. \quad (12)$$

This number comes from the requirement that there should be two families, related by transposition and intersecting in a family arising from the Diţă construction in such a way that the two sheets span the whole tangent space—with its dimension given by the linearised calculation—when they intersect. We feel quite confident that this is true, but more to the point we feel that the mere fact that we were at all able to put forward a concrete conjecture suggests that there is a pattern here—we are not very close to a full solution of the problem for general N , but we do feel that we have a right to expect that eventually a solution will be found, in reasonably compact form.¹

That is to say, however odd the conjecture (12) may seem, we feel that it represents the beginning of a clear cut answer to the question posed in the title.

CONCLUSION

A charge that has been raised against quantum mechanics is that of boring repetition: one might feel that the shape of the space of possible states should depend in an interesting way on the physical nature of the system, but in fact quantum mechanics uses the same old Hilbert space for everything [28]. Perhaps what we have seen is a possible answer to this. The existence of pairs of complementary bases has an elegant interpretation in terms of the shape of the convex body of all possible states. And in this regard that shape does depend dramatically on the number theoretical properties of the dimension of the Hilbert space.

But the dimension of the Hilbert space of a physical system is a property that can be measured, or at least be bounded from below by measurements [29, 30]. It has even been argued that the dimension of the Hilbert space is a

¹ Actually the argument in our published paper [27] is quite a bit stronger than the one I present here: here I tell the story as I knew it during the Växjö meeting.

candidate for the elusive role of something that goes on in between preparation and measurement [31]. If we accept this, and if the results above have convinced us that the shape of the space of states does depend in an interesting way on the dimension of Hilbert space, then the charge against quantum mechanics falls. The shape and feel of the body of quantum states does depend on the physical nature of the system.

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